1-Octanol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.46e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.80e-01

Confidence level: 8.18e-01

Nearest Neighbors from the Training Set

Image not found
1-Octanol
Measured: 4.15e-03
Predicted: 4.46e-03

Image not found
6-Methyl-1-heptanol
Measured: 4.97e-03
Predicted: 6.31e-03

Image not found
2-Ethyl-1-hexanol
Measured: 6.02e-03
Predicted: 6.58e-03

Image not found
1-Nonanol
Measured: 9.71e-04
Predicted: 1.41e-03

Image not found
1-Heptanol
Measured: 1.44e-02
Predicted: 1.44e-02